Benzene

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 10.0

Global applicability domain: Inside

Local applicability domain index: 6.82e-01

Confidence level: 7.86e-01

Nearest Neighbors from the Training Set

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1,2-Dibromoethane
Measured: 15.1
Predicted: 13.4

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Thiophene, 3-methyl-
Measured: 5.25
Predicted: 7.49

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Thiophene
Measured: 8.91
Predicted: 6.68

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Isoprene
Measured: 20.0
Predicted: 15.6

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Nitrobenzene
Measured: 4.68
Predicted: 8.00